

Amendments to the Specification

Please add the following paragraph to the specification at page 1, line 8:

A source code listing of the preferred computer program (algorithm) entitled "METHOD AND SYSTEM FOR PREDICTING PHARMACOKINETIC PROPERTIES" is part of this application and disclosure, and the source code and computer program are hereby incorporated herein in their entirety for all purposes. The listing consists of two files: "2dfp.spl" (14 kilobytes) created May 30, 1999 and "2dfp_Abs.spl" (15 kilobytes) created September 20, 1999. The source code listing is being submitted as a computer program listing appendix on the two accompanying identical sets of compact discs (each set marked "Copy 1" or "Copy 2," as appropriate, and consisting of one disc), created on or about March 18, 2004, in accordance with 37 C.F.R. §§ 1.52(e), 1.77(b)(4), and 1.96(c), all of which discs and the files thereon hereby being incorporated herein in their entirety for all purposes. The electronic name of the disc of Copy 1 is "METHOD_AND_SYSTE" and the electronic name of the disc of Copy 2 is "METHOD_AND_SYSTE." Each of the discs bears an external label with the title "METHOD AND SYSTEM FOR PREDICTING PHARMACOKINETIC PROPERTIES COMPUTER PROGRAM LISTING APPENDIX" as well as the other information required by 37 C.F.R. § 1.52(e)(6). A separate transmittal letter for the discs, in accordance with 37 C.F.R. § 1.52(e)(3)(ii), accompanies this application.

Please replace the heading set forth at page 4, line 11 by the following:
Brief Description of Drawings.

Please replace the paragraph beginning at page 5, line 27, with the following amended paragraph:

The term "internally developed macro" as used herein, refers to an internally developed ~~Sybyl~~ SYBYL™ Programming Language (SPL) code.

Preferable internally developed macro is as described in ~~Working Examples 4 and 5~~ the Computer Program Listing Appendix set forth on the accompanying CDs accompanying this Response.

Please replace the paragraph beginning at page 6, line 20, with the following amended paragraph:

(b) The prepared 2D-structure of a molecule can be imported into molecular modeling software such as SYBYLTM as a MOL2 format. 2D-fingerprints can be constructed by the use of internally developed macro script 2dfp.spl or 2dfp_abs.spl; written in SYBYLTM Programming Language (SPL) implemented in SYBYLTM, or by manually counting the number of the atoms/fragments or substructures. The macro program converts 2D-structures stored in the molecular database as a MOL2 format into a SYBYLTM line notation (SLN) format. Subsequently, the macro searches each SLN for the substructures potentially related to a pharmacokinetic property that match the queries described in the macro (as ~~shown in Working Example 4~~ included in the Computer Program Listing Appendix, set forth on the accompanying CDs), wherein the queries are predefined as the substructures (20 to 80 atoms/fragments). Finally the macro enumerates the substructure counts, and records them as 2D-fingerprints.

Please delete the source code listing beginning at page 14, line 11 and ending at page 23, line 7.

Please delete the source code listing beginning at page 23, line 18 and ending at page 25, line 11.